

Ocimene (E)  
3779-61-1 | DTXSID8040567

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.40e-10 cm3/molecule\*sec

Global applicability domain: Inside

Local applicability domain index: 3.10e-01

Confidence level: 8.96e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ocimene (E)</div> <div>Measured: 2.52e-10</div> <div>Predicted: 2.40e-10</div>	<div>Image not found</div> <div>beta-Ocimene</div> <div>Measured: 2.52e-10</div> <div>Predicted: 2.40e-10</div>	<div>Image not found</div> <div>Myrcene</div> <div>Measured: 2.15e-10</div> <div>Predicted: 2.05e-10</div>
<div>Image not found</div> <div>Linalool</div> <div>Measured: 1.60e-10</div> <div>Predicted: 1.65e-10</div>	<div>Image not found</div> <div>D-Limonene</div> <div>Measured: 1.71e-10</div> <div>Predicted: 1.73e-10</div>	<div>Image not found</div> <div>3-Methylidene-6-(propan-2-yl)cyclohexene</div> <div>Measured: 1.68e-10</div> <div>Predicted: 1.63e-10</div>